

## Article

# Improving the Carbon Capture Efficiency for Gas Power Plants through Amine-Based Absorbents

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**Abstract:** Environmental concern for our planet has changed significantly over time due to climate change, caused by an increasing population and the subsequent demand for electricity, and thus increased power generation. Considering that natural gas is regarded as a promising fuel for such a purpose, the need to integrate carbon capture technologies in such plants is becoming a necessity, if gas power plants are to be aligned with the reduction of CO<sub>2</sub> in the atmosphere, through understanding the capturing efficacy of different absorbents under different operating conditions. Therefore, this study provided for the first time the comparison of available absorbents in relation to amine solvents (MEA, DEA, and DEA) CO<sub>2</sub> removal efficiency, cost, and recirculation rate to achieve Climate change action through carbon capture without causing absorbent disintegration. The study analyzed Flue under different amine-based solvent solutions (monoethanolamine (MEA), diethanolamine (DEA), and methyldiethanolamine (MDEA)), in order to compare their potential for CO<sub>2</sub> reduction under different operating conditions and costs. This was simulated using ProMax 5.0 software modeled as a simple absorber tower to absorb CO<sub>2</sub> from flue gas. Furthermore, MEA, DEA, and MDEA adsorbents were used with a temperature of 38 °C and their concentration varied from 10 to 15%. Circulation rates of 200–300 m<sup>3</sup>/h were used for each concentration and solvent. The findings deduced that MEA is a promising solvent compared to DEA and MDEA in terms of the highest CO<sub>2</sub> captured; however, it is limited at the top outlet for clean flue gas, which contained 3.6295% of CO<sub>2</sub> and less than half a percent of DEA and MDEA, but this can be addressed either by increasing the concentration to 15% or increasing the MEA circulation rate to 300 m<sup>3</sup>/h.

**Keywords:** process technology description of different amine solvents; amine-based chemical solvent using monoethanolamine (MEA); degradation of MEA and other solvents; diethanolamine (DEA) solvent; methyldiethanolamine (MDEA)



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## 1. Introduction

A considerable amount of attention has been focused on our planet due to the conceivable outcomes of climate change, which is a result of the energy generated from fossil fuel emissions and greenhouse gases such as CO<sub>2</sub>. Therefore, the number of CO<sub>2</sub> capture technologies has increased significantly due to their flexibility and design, efficacious cost, and proficient application [1,2]. In addition, flue gas is released into the environment from diverse industries, including power generation, the petrochemical industry, and refinery gases [3]. The definition of flue gas is a blend of combustion products, including carbon dioxide, particulates, water vapor, heavy metals, and acidic gases, generated from indirect (gasification and pyrolysis) intermediate synthesis gas or the oxidation of radial distribution functions (RDF) or generated directly (incineration) [4,5]. In this research, we will examine which of the chemical solvents of monoethanolamine (MEA), diethanolamine (DEA), and methyldiethanolamine (MDEA) are best able to produce good, low-cost outcomes; low amine degradation; and losses to remove or capture CO<sub>2</sub> from flue gases. Carbon dioxide must be separated from the gases and other vapors by using absorption technology, which

is used to remove carbon dioxide from flue gases by employing liquid solvents (e.g., MEA, MDEA, DEA, etc.) for this purpose. This was conducted in this study by a simulation program (ProMax) and there were two scenarios employed to compare amine solvents from previous study [6]. Currently, chemical solvents using absorption process consider use the technology of the post-combustion CO<sub>2</sub> capture technologies, considered one of the best technology for capturing CO<sub>2</sub>, in addition to pre-combustion capture that has been used to remove CO<sub>2</sub> and H<sub>2</sub>S from natural gas components in a refinery [5–7].

This study also presents trade-off option of CO<sub>2</sub> capture versus amine recirculation required and cost for amine solvents (MEA, DEA, and MDEA). Therefore, the most significant problem which must be determined and considered is the percentage of oxygen in the flue gas, which is affected by caused degrade of the amine solvents. These solvents cause oxidative degradation and should prevent it and limit it to around 5 to 10 ppm [8]. Additionally, as a UK report, the highest emission came from power generation, which is shown in Table 1. Therefore, choosing a power generation station represents the best source of CO<sub>2</sub>. The total emission of CO<sub>2</sub> by power stations in the UK annually given in a British petroleum (BP) report is 65.2 million tons, which is a huge number, as shown in Table 1 [5].

**Table 1.** Greenhouse gas emissions in 1990–2018 in the UK on an annual basis (CO<sub>2</sub> in million tons).

Years	1990	1995	2000	2005	2010	2015	2017	2018
Energy supply	242.1	210.3	204.0	219.1	197.3	137.6	106.0	98.3
from power stations	203.0	163.0	158.7	173.1	157.3	104.1	72.4	65.2

## 2. Theory (Literature Review)

### 2.1. Background

There are two significant points that should be considered before capture CO<sub>2</sub>, which are

- How to deal with the huge amount of carbon dioxide from fossil fuels formed during combustion;
- How to grip impurities of the stream in flue gas.

The impurities in flue gas may contain sulfur and nitrogen oxides, particulate matter, and water vapor. The combustion of the fuel source will produce various amounts of impurities and changes, depending upon the fuel source. It is crucial to know the fundamental mechanisms behind CO<sub>2</sub> and to prevent impurities and the formation of impurities during the combustion of fossil fuel [9]. The common reactions taking place during combustion can be applied to any fuel for CO<sub>2</sub> formation, as follows in Equations (1) and (2) [9]:



This is uncompleted combustion,



This is a complete combustion.

It should be noted that, when using natural gas instead of coal, the emissions of carbon dioxide will be significantly reduced and the coal will emit more nitrogen and sulfur dioxide because it will contain more impurities, rather than natural gas. Acid rain is caused by nitrogen and sulfur oxides, which are the main contributors to its formation. There is an advantage of employing some technologies for capturing CO<sub>2</sub>, such as oxy-combustion, chemical looping combustion, and pre-combustion, which is the creation of an environment for combustion without impurity precursors, such as H<sub>2</sub>, S, N, and N<sub>2</sub>. However, there are certain amounts of inherent nitrogen and sulfur in fuel, so complete

impurity removal is not possible, and it cannot be considered as a perfect fuel. In addition, this impurity of combustion depends on the process that is used to treat the fuel before use in burning. In common cases of CO<sub>2</sub> capture, the impurities are removed from flue gas before capture is applied. Finding ways to handle the large quantity of CO<sub>2</sub> produced by burning fuel in power stations, whatever the source of fuel, is a big challenge [9]. In the different power plants in Hebei Province, China, as shown in Table 2, the raw coal had a high emission value of about 900 to 1000 g per KW/h, which is double the amount of oil and gas that was emitted. Moreover, it needs excess oxygen more than other fuels to complete combustion, which is considered a challenge when using chemical solvents to capture CO<sub>2</sub>, increasing the degradation when amine solution is used [10,11]. However, the consumption of fuel per KW/h for oil and natural gas represents less than one third of the consumption of raw coal required to generate power. Currently, commercial CO<sub>2</sub> capture systems have a maximum capacity of about 800 t/d CO<sub>2</sub>, which means that the capture process emits approximately ten times less than that in a power plant. Therefore, it is appropriate to begin discussing the various CO<sub>2</sub> capture approaches and their associated technologies, such as post-combustion, pre-combustion, oxy combustion, and chemical looping combustion [7,9,10,12,13].

**Table 2.** The emission of flue gases from different power plans in Hebei Province, China.

Fuel Type	Fuel per Kilowatt-Hour	PM <sub>2.5</sub> (mg/m <sup>3</sup> )	SO <sub>2</sub> Emission (mg/m <sup>3</sup> )	CO <sub>2</sub> Emission (g)	NO <sub>x</sub> Emission (mg/m <sup>3</sup> )	CO Emission	O <sub>2</sub> %
Coal	290–340 g	20–30	50–200	900–1000	100–200	1800–2000	9
Oil	80–90 g	20–30	50–100	400–450	100–200	1800–2000	3.5
Natural gas	70–80 g	5–20	35–50	400–450	100–150	1800–2000	3.5

On the other hand, rather than the amount of CO<sub>2</sub> emitted into the atmosphere by many industries, the chemical and the physical properties of the CO<sub>2</sub> should be studied to learn about it and how it behaves. Therefore, Table 3 illustrates the physical and chemical properties of CO<sub>2</sub> [14], and Table 1 shows the properties of CO<sub>2</sub> that used in amine absorption come out from ProMax in Appendix A.

## 2.2. Process Technology Description of Different Amines

Amine processing includes two major processes of absorption and separation. When the CO<sub>2</sub> is absorbed by a lean amine aqueous solution solvent through an absorption process, the equipment used is called an absorber. In addition, the process in which the CO<sub>2</sub> is separated from aqueous solution by applying heat is called a separation or regeneration process, and the equipment employed is called a regenerator or stripper [15]. Moreover, the treatment occurs at an absorber at high pressure and at a low temperature, while at the stripper, there is a low pressure and high temperature between 100 and 120 °C [13,16]. There are some arguments about the stripping temperature, which varies between 120 and 150 °C [8,17], 95 and 135 °C [18], and 120 and 140 °C [15]. Therefore, the system includes heat, a cooling source, and a compressor to raise the pressure of flue gas before it enters the absorber. Furthermore, the system includes a pump to circulate the lean solution and rich amine [13,15,16]. In absorption, the following steps occur [19]:

- CO<sub>2</sub> dissolves into the absorbent;
- A low temperature is required to ensure a high rapport for the absorption of CO<sub>2</sub>;
- The distribution of CO<sub>2</sub> will occur between the gas–liquid interface and the bulk gas;
- The CO<sub>2</sub> will react with the amine in the solution.

**Table 3.** The physical and chemical properties of CO<sub>2</sub>.

Property	Value and Unit
Molecular weight	44.01 g/mol
Critical density ( $\rho_c$ )	0.468 g/cm <sup>3</sup> or 468 g/L or 468 kg/m <sup>3</sup>
Critical pressure ( $P_c$ )	72.85 atm (7383 kPa)
Critical temperature ( $T_c$ )	31.04 °C
Triple point pressure	5.185 bar
Triple point at 5.1 atm (518 kPa)	−56.5 °C
Sublimation point at 1 atm (101.3 kPa)	−78.5 °C
Gas density at 0 °C and 1 atm (101.3 kPa)	1.976 g/L
Liquid density at 0 °C and 1 atm (101.3 kPa)	928 g/L
25 °C and 1 atm CO <sub>2</sub> (101.3 kPa)	0.712 v/v
Solid density	1560 g/L
Specific volume at 1 atm and 21 °C	0.546 m <sup>3</sup> /kg
Latent heat of vaporization at the triple point (−78.5 °C)	
At 0 °C	353.4 J/g
231.3 J/g	
Viscosity at 25 °C and 1 atm CO <sub>2</sub> (101.3 kPa)	0.015 cP (mPas)
Solubility in water at 0 °C and 1 atm (101.3 kPa)	
25 °C and 1 atm (101.3 kPa)	0.3346 g CO <sub>2</sub> /100 g-H <sub>2</sub> O or 1.713 mL CO <sub>2</sub> /mL-H <sub>2</sub> O at 0 °C
0.1449 g CO <sub>2</sub> /100 g-H <sub>2</sub> O or 0.759 mL CO <sub>2</sub> /mL-H <sub>2</sub> O at 25 °C	
Heat of formation at 25 °C, $\Delta H$ gas	0.1372–393.5 kJ/mol

The flue gas results from burning fossil fuel in power stations and represents approximately 3–20% of gas emitted. It is fed into an absorption column, needed to cool the temperature of flue gas to below 50 °C or about 47–50 °C, due to the high temperatures of the exhaust gas of power generations [17]. After the flue gas has been cooled by an exchanger, such as cooling water and a fan cooler, it will enter the absorption tower or so-called absorber column and pass through it from bottom to top, in which approximately 86–90 vol.% of the CO<sub>2</sub> is absorbed by solvent [5,13,15,20] and amine absorbs the carbon dioxide at 40–75 °C [18]. In addition, the absorbent or solvent enters the column from the top side of the tower and moves down to the bottom. In the meantime, the flue gas which contains acid gas will react with the solvent and usually has a temperature of nearly 40 °C. Through this process, lean amine is converted into rich amine, which means that CO<sub>2</sub> is absorbed by aqueous amine solution. Secondly, heat is released as a result of the absorbed CO<sub>2</sub> and the temperature of the solvent is increased due to the exothermic reaction, which is a kind of reversible reaction. At the bottom of the absorber, the CO<sub>2</sub>-rich stream will be collected at a required level, to prevent untreated gas from escaping from the desorber tower and, for safety reasons, to prevent the stripper tower caps and trays from being damaged due to the high differential pressure between the regenerator and absorber.

The purified gas emitted out into the atmosphere is washed by water at the top of the absorber to cool the top of the tower, prevent evaporation of the amine solution, and mitigate the loss of solvent [9,13,15,17]. Furthermore, the loading is varied from 0.1 to 0.45 mol CO<sub>2</sub>/mol amine, depending on the lean and rich solvent (generally, lean and rich solvent CO<sub>2</sub> loading of 0.1–0.2 mol CO<sub>2</sub>/mol MEA and 0.4–0.5 mol CO<sub>2</sub>/mol MEA, respectively) and on several other factors, which are

- The increasing or decreasing amine flow rate;
- The increasing/decreasing concentration of amine, considering the factors of corrosion that are caused by amine and the amount of CO<sub>2</sub> that will be absorbed;
- The loading is defined as the total amount of CO<sub>2</sub> absorbed by amine and can be described as in Equations (3) and (4) [16,21]:



$$\text{Loading} = \frac{\text{Moles of all CO carrying species}}{\text{Moles of all MEA carrying species}} \quad (3)$$

$$\text{Loading} = \frac{[\text{MEA}] + [\text{MEA}^+] + [\text{MEACOO}^-]}{[\text{CO}_2] + [\text{HCO}_3] + [\text{CO}_3^{-2}] + [\text{MEACOO}^-]} \quad (4)$$

The absorber column or tower includes trays and is different, depending on the solvent used for the capturing process [15]. Figure 1 illustrates the different types of amine aqueous solutions with the number of trays used in each solvent [15].

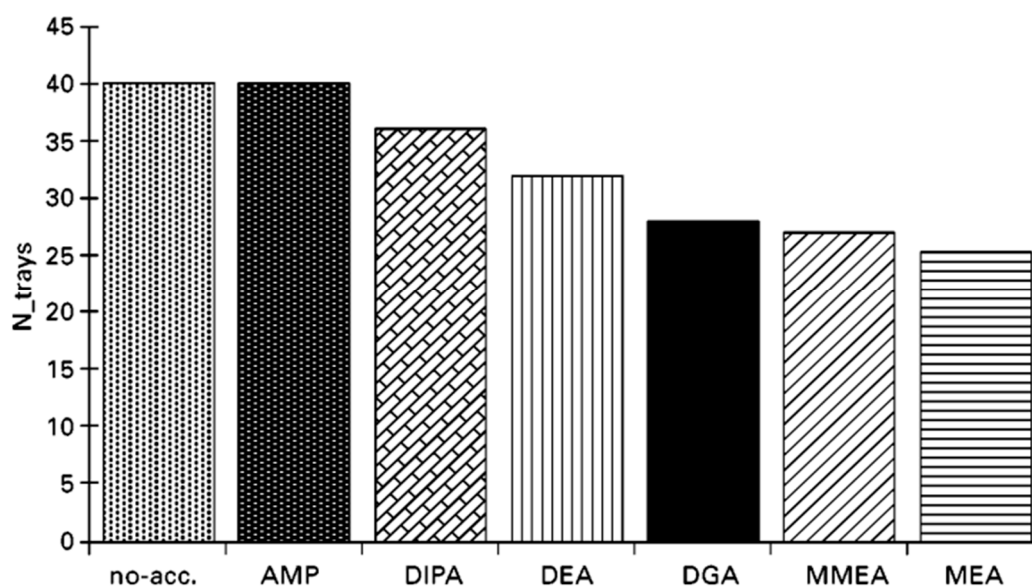


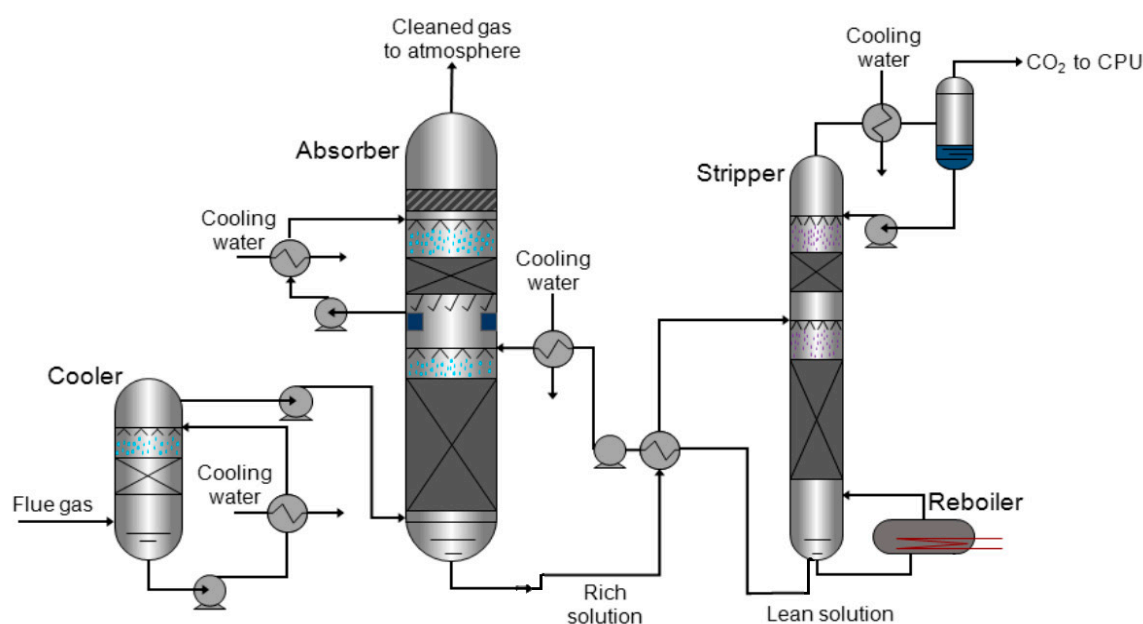
Figure 1. Number of trays required for CO<sub>2</sub> absorption in an amine's aqueous solution.

The rich amine solution leaves via the bottom of the absorber, which is then heated to about 100 °C across the amine–amine exchanger (lean/rich amine heat exchanger). It is fed to the top side of a stripping column or regenerator, in order to minimize the heating energy cost of the rich solution, which is required before it enters the stripper to avoid widely different temperatures between the solvent and regenerator. The flow that happens between the absorber and stripper occurs due to the different pressures between them, which is quite high, being about 15–20 times greater than the regenerator pressure [21]. In the desorption column, the following occur [19]:

- To ensure a lower relationship for the absorption of CO<sub>2</sub>, the temperature be should be high;
- To ensure that CO<sub>2</sub> will be released, chemical equilibria should occur;
- The desorption process is endothermic; therefore, to maintain the high temperature, heat must be applied to the absorbent.

Where further heated, a supply at the bottom of the stripper is required to increase the temperature to 120–140 °C by using a steam reboiler which is generated for this purpose or the power plant will become exhausted. The operating pressure for a stripper is nearly 1.5–2 bar and it is formed of a packed column which has a kettle reboiler [5,15,21]. The rich solution or stable product that formed in the absorber and the CO<sub>2</sub>, which was absorbed by the solvent, will be recovered at the regenerator column; then, CO<sub>2</sub> will be released from the absorbent inside the stripper at a high temperature of 100–120 °C, due to the equilibrium isotherm and loading (mole of CO<sub>2</sub>/mole of amine) transfer from higher (rich amine) to lower loading (lean amine means amine that had taken off the CO<sub>2</sub>); that is why the solvent-recovering energy cost is high. The lean solution at the bottom of the regenerator

is circulated back to the absorption tower after passing through the heat exchanger and cooler [13,15,16]. The gas consisting of a mixture of water vapor and CO<sub>2</sub> with some evaporated amine travels out of the top of the stripper and enters a cooler to cool it. Then, it is fed into a flash drum and the acid gas, which is CO<sub>2</sub> from condensate water, and amine are physically separated, no matter the kind of amine. Finally, CO<sub>2</sub> is compressed and transported for sequestration. Figure 2 shows a schematic diagram of the amine-based chemical absorption process [8,17].



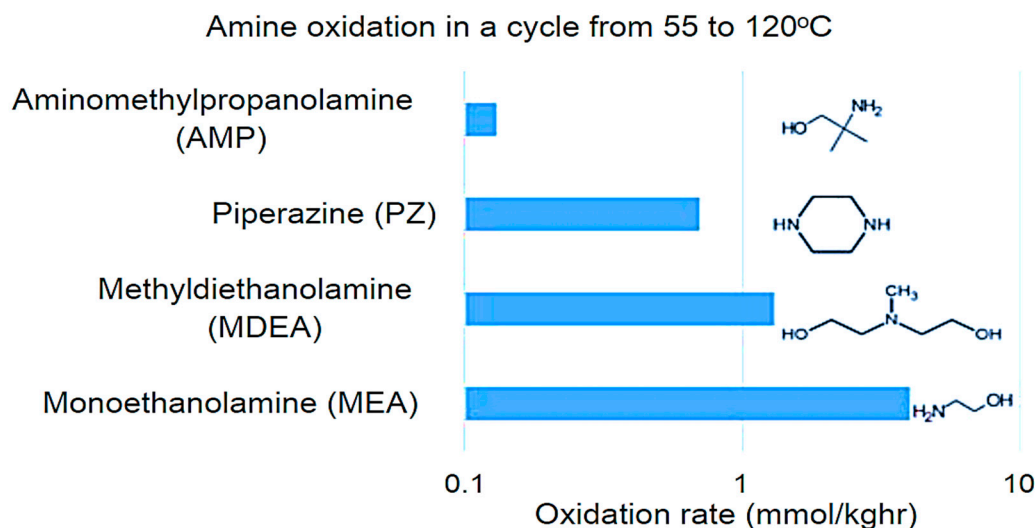
**Figure 2.** Schematic diagram of the chemical absorption process used for capturing CO<sub>2</sub> with solvent process regeneration.

### 2.3. Amine-Based Chemical Solvent Using Monoethanolamine (MEA)

Amines are officially derivatives of ammonia, and where one or more hydrogen atoms have been displaced by an organic substituent, such as an alkyl group, these amines called alkylamines [22]. MEA is one of the most important absorption liquids and is the least expensive. It can be produced in large quantities from ethylene oxide and ammonia reactions. The Acid Dissociation Constant (pKa) is close to a primary amine. Therefore, it has a very good viscosity and an excellent average rate of absorption of CO<sub>2</sub>, with an over-average normalized ability [19]. An amino group is the perfect group for absorbing CO<sub>2</sub> and provides enough alkalinity. It is commonly dissolved so that CO<sub>2</sub> chemically reacts with alkanolamines. One of the most crucial advantages of alkanolamines is that, structurally, at least one hydroxyl group is contained in them. Due to this, it can help to raise the solubility in aqueous solutions and mitigate the vapor pressure [10]. Monoethanolamine (MEA) is considered one of the most general alkanolamine groups and is widely used. It has been used for over 75 years to remove CO<sub>2</sub> and H<sub>2</sub>S from natural gas and flue gas [23]. Due to MEA having a high-water solubility, high cyclic capacity, and considerable kinetic rates of absorption-stripping at a low CO<sub>2</sub> concentration, it is considered to be a standard sorbent [8].

The capacities of chemical and physical MEA absorption are affected by the pressure, temperature, concentration of aqueous MEA, and presence of additional gases, which means impurities [22]. The weight % concentration of monoethanolamine varies from 15 to 35%, depending on the process and 0.45 CO<sub>2</sub> moles/mole amine (324 g CO<sub>2</sub>/kg MEA), so the lean and rich amine solvent loading can vary from 0.242 to 0.484 CO<sub>2</sub> moles/mole amine, respectively [2,9,22]. However, others have reported that monoethanolamine can remove around 90% and 30 wt.% MEA solution with optimum lean amine solvent loading

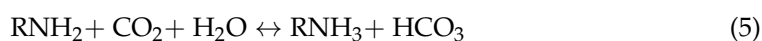
of nearly 0.32–0.33 mol CO<sub>2</sub>/mol MEA and a requirement of thermal energy of 3.45 GJ/ton CO<sub>2</sub> [2]. Figure 3 [24] shows the chemical structure of primary amine and Table 4 illustrates the typical characteristics of amine solvents for MEA and other amines used for CO<sub>2</sub> absorption [8,15,16,24,25].



**Figure 3.** The oxidation rate of general amines with cycling from 55 to 120 °C.

There are two major amine technologies used to treat flue gas. Kerr-McGee/ABB Lummus Crest was the first commercial technology, developed by Mitsubishi Heavy Industries with the Kansai Electric Power Company in the 1990s. This technology is operated with cogeneration systems and boilers that have a range of fire fuels. The concentration of aqueous amine solution MEA is about 15–20%. However, in this process, the flue gas should contain limited sulfur dioxide, as well as tolerate a reasonable amount of oxygen. Furthermore, in 1978, the first Kerr-McGee/ABB Lummus Crest technology in Trona (California) recovered CO<sub>2</sub> from flue gas, with a production value of 800 t/day of CO<sub>2</sub>. The most crucial advantages are the low amine losses, low heat required for regeneration, and low amine degradation due to the additives and inhibitors used in this technology [15].

The second technology is the Fluor process, which was developed by Fluor Daniel from Dow Chemical in 1989. Using a 30 wt.% of MEA solvent, the Kerr-McGee/ABB Lummus Crest process uses additives and inhibitors to prevent equipment corrosion and degradation. The Fluor Daniel process has mainly been used to remove exhaust gases and has been employed in more than 20 plants worldwide. For example, in Lubbock, Texas, the plant has a capacity rate of about 1200 t/day of CO<sub>2</sub>. This technology can recover between 85 and 95% of CO<sub>2</sub> from flue gas, with the purity reaching 99.95% [15,19,21]. The two most fundamental reactions of amines are shown in Equations (5) and (6) [22,26,27]:



Finally, the temperature which causes the MEA to become exposed to thermal degradation is 120 °C and is considered one of the main drawbacks in comparison to oxidation, so inhibitors should be used to avoid it [20].

**Table 4.** Typical characteristics of amine solvents employed for monoethanolamine (MEA) and other amines used for CO<sub>2</sub> absorption.

Amine	Monoethanolamine (MEA)	Diethanolamine (DEA)	Diglycolamine (DGA)	Methyldiethanolamine (MDEA)	Diisopropanolamine (DIPA)
Typical Concentration range recommended (wt.%)	13–20 15–25	25–30 20–40	50–60 50–65	35–55	20–40
Solvent loading (mole/mole)	0.3	0.3–0.7	0.35	0.45	0.45
Heat of regeneration (MJ/kg CO <sub>2</sub> )	2	1.5	2	1.3	1.5
Chemical formula	C <sub>2</sub> H <sub>7</sub> NO	C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub>	C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub>	C <sub>5</sub> H <sub>13</sub> NO <sub>2</sub>	C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub>
Boiling point (°C)	171	269	221	247	249
Molecular weight (g/mol)	61.08	105	105	119.16	133

#### 2.4. Degradation of MEA and Other Solvents

The MEA degradation rate is nearly 1.5 kg/ton CO<sub>2</sub> whatever the type of degradation [2,20]; therefore, degradation has several types, and two major types will now be discussed.

##### A. Oxidative degradation

Oxidation degradation occurs because of flue gas containing oxygen in the absorber tower. Neither a high temperature nor CO<sub>2</sub> is required for oxidative degradation. This is a major issue for capturing CO<sub>2</sub> in the flue gas, and the concentration of oxygen varies between 3 and 5% in the gas stream. It mainly occurs in the absorber, at 40–70 °C [8]. In addition, according to a study conducted at the University of Texas, the degradation can be controlled by the mass transfer of oxygen under industry conditions, where the degradation rate is nearly 0.29–0.73 kg of MEA/ton of CO<sub>2</sub>. Furthermore, loss of the solvent and the formation of heat-stable salts are also caused by oxidative degradation, and to prevent this, inhibitors are added to the system [21,23]. The products, such as aldehydes, organic acids, and ammonia, are formed by an oxidative degradation chain of amine solvent starting with MEA. In the second step, the acids are formed (heat-stable salts), leading to mitigation of the capacity rate of the absorption of CO<sub>2</sub> by the solvent. These acids react with the absorbent MEA, leading to the production of amide compounds [8,23]. Table 5 shows the oxidative degradation compounds formed from MEA [8,23].

**Table 5.** The formation of compounds from the oxidative degradation of MEA.

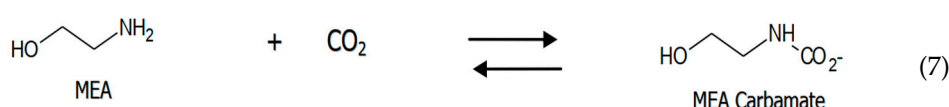
Solvent	Compounds
MEA	inorganic compounds (NH <sub>3</sub> , NO <sub>2</sub> <sup>−</sup> , NO <sub>3</sub> <sup>−</sup> )
	Organic acids (HCOO <sup>−</sup> , CH <sub>3</sub> COO <sup>−</sup> , HOCH <sub>2</sub> COO <sup>−</sup> , (C <sub>2</sub> O <sub>4</sub> ) <sup>2−</sup> )
	Amides (oxamides, HEF, formamides,)
	cyclic compounds (HEPO-3, HEPO-2, HEI, HEP, DMPz)
	Aldehydes (CH <sub>3</sub> CHO, HOCH <sub>2</sub> CHO, CH <sub>2</sub> O)
	Amines (MAE, methylamines, BHEEDA, MEA-urea)

Diethanolamine is formed by oxidizing primary and tertiary amines; however, a large amount of diethanolamine is also produced by oxidizing MDEA, as shown in Figure 3 [19].

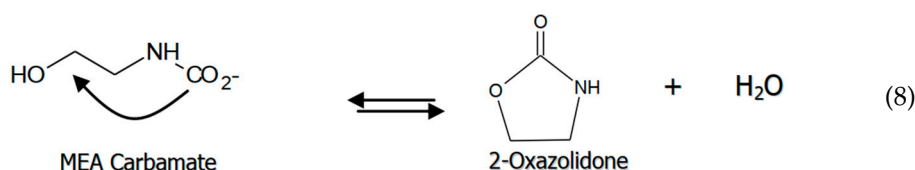
#### B. Thermal degradation of MEA and other solvents (polymerization of Carbamate):

Polderman was the first person to propose the mechanism of the polymerization of carbamate of MEA in 1955 [28]. The polymerization of carbamate occurs in the stripper column at a high temperature and over a long period of time [21]. The thermal degradation increases when the temperature is increased in the stripper column, where the degradation rate of MEA or any solvent will be 2.5–6% per week at a temperature of about 135 °C [16]. The polymerization of carbamate causes an increased amine solution viscosity, loss of carbon dioxide's absorption capacity, increased corrosion, and foaming [28]. The mechanism of degradation is as follows.

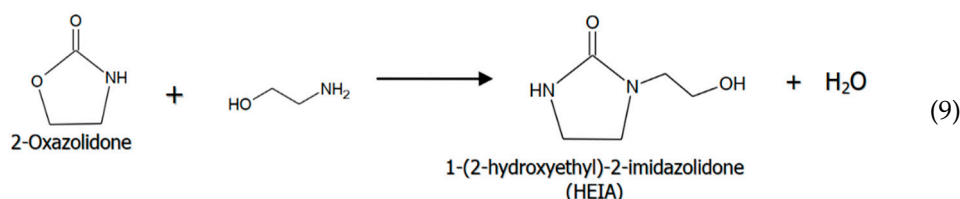
First, the reaction occurs at the absorber with CO<sub>2</sub>, and CO<sub>2</sub> associates with MEA to form carbamate of MEA, as shown in Equation (7) [28]:



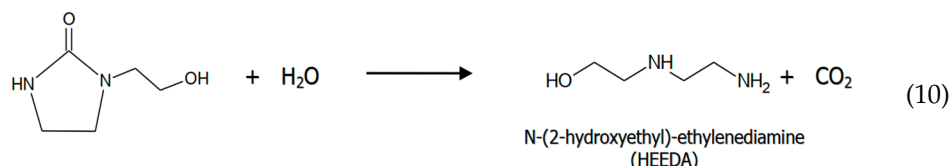
Then, at the stripper, the reaction is generally reversed; however, for some statuses, 2-oxazolidone will form due to the cyclizing of MEA carbamate, and this reaction type is also reversible, as shown in Equation (8) below [8]:



Furthermore, the 2-oxazolidone will react with one mole of monoethanolamine to form 1-(2-hydroxyethyl)-2-imidazolidone and is referred to as HEIA. Equation (9) shows the reaction [29]:



After that, the HEIA will react with water (hydrolyze) to form HEEDA, which is N-(2-hydroxyethyl)-ethylenediamine, as illustrated in Equation (10) [28]:



These four types (HEEDA, dihydroxy ethyl urea, 2-oxazolidone, and HEIA) of formation are the major products of thermal degradation [29].



### 2.5. Diethanolamine DEA Solvent

DEA is often used an abbreviation for diethanolamine, and it is an organic component that has both a Dialcohol and a secondary amine. In addition, a Dialcohol contains two hydroxyl groups in its molecule [19,30]. Diethanolamine, like other alkanol amines, rules as a weak base [24].

DEA is an inexpensive solvent due to its wide use in many industries, and it is especially used for removing CO<sub>2</sub> and H<sub>2</sub>S in natural gas that has rapidly reacted, where the selectivity is high (between other and acid gases), and for the reversible reaction process at the absorber column. Furthermore, the operation conditions can be a low heat reaction (around 70 kJ/mol CO<sub>2</sub>) and low pressure [30]. One of the most common disadvantages is the presence of SO<sub>2</sub> and O<sub>2</sub> in flue gas, causing solvent degradation (which should be less than 10 ppm). The presence of O<sub>2</sub> in flue gas causes the oxidation of DEA and leads to increased degradation [10]. The concentration of diethanolamine varies, depending on the amount of CO<sub>2</sub> to absorb. In approved industries, the concentration has been shown to be between 25 and 35% and lean amine (DEA) loading is set at 0.1 mol CO<sub>2</sub>/mol DEA [30], whereas the rich amine of diethanolamine loading is 0.4 mol CO<sub>2</sub>/mol DEA, as illustrated in Figure 4 [5].

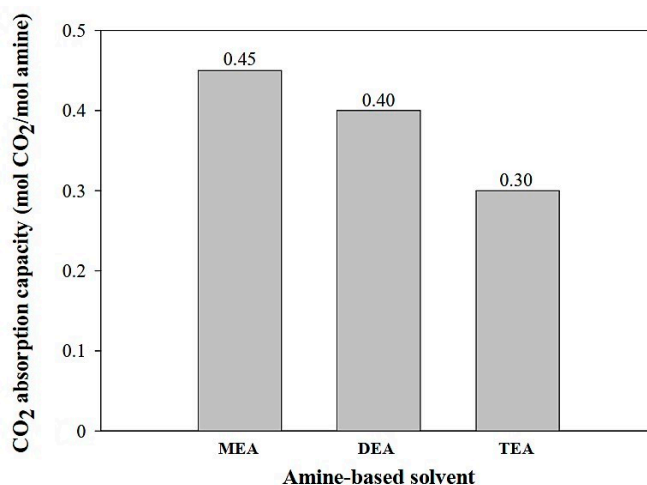


Figure 4. The different types of amine with the capacity to absorb CO<sub>2</sub>.

However, the mechanism of degradation of DEA is a similar to that of MEA [28]. Consequently, the products produced after degradation are Tris-hydroxyethyl ethylenediamine called THEED, Bis-hydroxyethyl piperazine (bis-HEP), MEA, Bis-(hydroxyethyl) glycine (Bicine), and polymers. Polymers are products produced when the DEA molecule reacts with THEED (ethylenediamines). Furthermore, the MEA product is obtained when the DEA molecule degrades in the presence of oxygen [31].

### 2.6. Methyldiethanolamine MDEA

MEDA is an abbreviation of N-methyldiethanol-amine and the chemical formula of it is C<sub>5</sub>H<sub>13</sub>NO<sub>2</sub> [15]. MDEA is considered a chemical solvent, so the chemical solvents have a characteristic during the absorption process, which is that the acid gas component in the solvent is bonded chemically [32]. The density of MDEA can range from 1 to 1.149 at a temperature roughly between 298 and 363.15 K with a concentration percentage between 23.8 and 60 wt.% [3]. MDEA can degrade at 119–129 °C [8]. Some of the advantages of MDEA are the need for only a low energy for regeneration due to the acidic gas reaction having a low enthalpy and the high capacity for the absorption of CO<sub>2</sub> [10]. In addition, the solution has a lower vapor pressure and corrosiveness, with a good chemical and thermal stability. On the other hand, there are some drawbacks, including the slow reaction with

carbon dioxide and low absorption capacity when the concentration of carbon dioxide is low [4].

MDEA has several advantages which make it a very popular solvent, including the fact that it is less aggressive, requires a low heat for the reaction with  $\text{CO}_2$ , is less corrosive, can be used in higher concentrations, has lower circulation rates, and is easier to regenerate [24].

The major determinate for the operating cost and capital cost is the circulation rate of the solvent, which is roughly proportional to the amount of acid gas to be removed. The process of gasification and flue gas treatment shown in Figure 5 is common and, as in the MEA process, the lean MDEA enters the absorber and reacts with acid gas to absorb some of the  $\text{CO}_2$  and  $\text{H}_2\text{S}$ , whereas bonding MDEA with  $\text{H}_2\text{S}$  takes place quicker than carbon dioxide. At the bottom of the absorber, the rich stream is pre-heated and enters the stripper/regenerator to regenerate the solvent by using the reboiler to break the bond of chemically reacted substances. The component of acid gas will be cooled through the cooler when exiting the top of the stripper column to condensate out the water for recycling purposes [32].

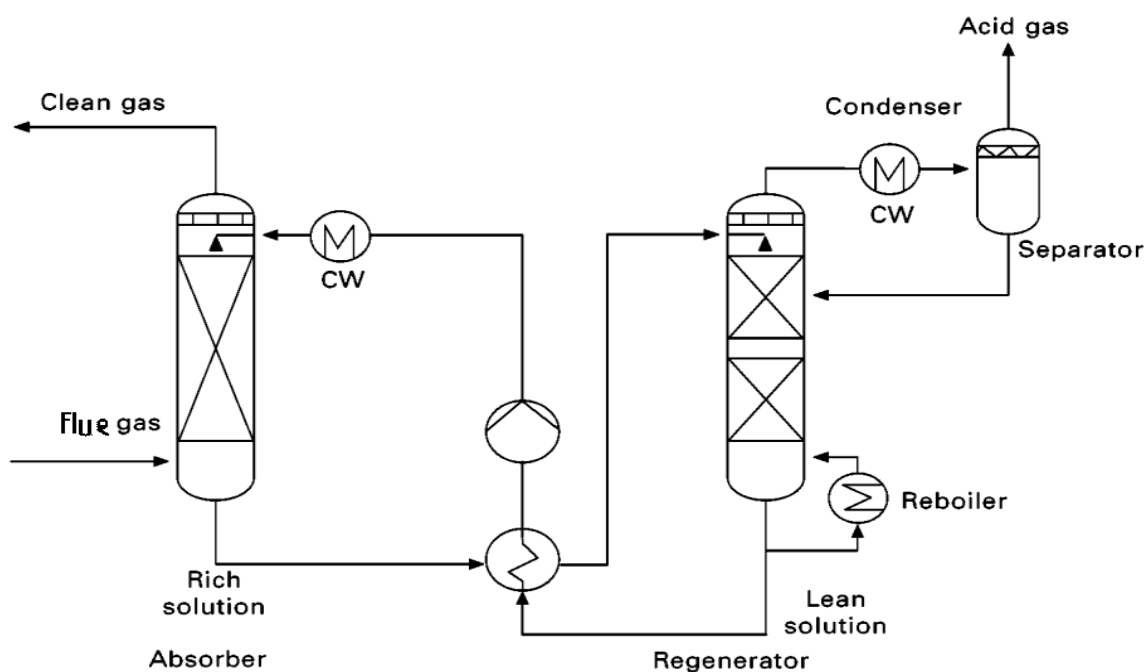


Figure 5. A flowsheet of the typical methyldiethanolamine (MDEA) process.

The degradation of MDEA will produce several products, which include dimers (degradation of DIPA-OX to diamines (“dimers”)), polymers (dimer reacts with a DIPA molecule), Monoisopropanolamine (MIPA) (occurs when oxygen reacts with a DIPA molecule), Triisopropanolamine (TIPA) (produced when amine degrades in the presence of oxygen in the flue gases to produce simpler amines, whilst these simpler amines will react with other base amines to produce complex amines), and others, such as DIPA and 1,1-Dioxidetetrahydrothiophene (Sulfolane) [31].

In 2008, Bedel assumed that there were several degradation pathways for MDEA, including hydrolysis, elimination reactions, disproportionation, and hemolytic splitting. Amino acid hydrolysis occurs in extrapolated conditions of a stripper and at a high temperature, which is a reasonable reason for degradation [28]. Under normal conditions of the regenerator, the common pathway for the degradation of MDEA involves the reaction of disproportionation, sometimes referred to as alkanolamine “scrambling”. Therefore, one molecule of dimethylethanolamine and triethanolamine is formed by replacing the methyl group in the MDEA molecule with another molecule of the ethanol group [8,28]. In this

process, a methyl group can be replaced with a hydrogen to form DEA, and this reaction can continue for amine degradation by the polymerization of carbamate [8,15,19].

### 2.7. Comparative Amines Solvent

Table 6 shows the comparatives of amine solvent, such as MEA, DEA, and MDEA as a rate, heat, and capacity of absorption, with the stability of solvent [19].

**Table 6.** Characterization properties of the solvents for popular amine solvents.

Absorbent	Rate of Absorption	Absorption Capacity CO <sub>2</sub>	Stability of Solvent	Heat of Absorption
Methyldiethanolamine (MDEA)	Low	High	High	Medium
Diethanolamine (DEA)	Medium	Medium	Medium	High
Monoethanolamine (MEA)	High	Medium	Low	High

### 3. Material and Method

This section highlights the framework involves in specifying the variables for solving absorber column using Promax, which was developed using a typical composition of the Flue gas from gas-powered power plant plants as obtained in Table 7.

**Table 7.** Flue gas feed compositions in mole%.

Compositions	Mole Percent (%)
N <sub>2</sub>	77
CO <sub>2</sub>	21
H <sub>2</sub> O	1.99
O <sub>2</sub>	0.01

The Amine Sweetening Peng Robinson (PR) was employed as the most compatible thermodynamic equation to handle the components listed in Table 7, when combined with Amine absorbent. The process was then followed by specifying the components in the Flue gas, followed by column convergence using MEA. This was then repeated at 300 m<sup>3</sup>/h as well as changing the absorbent type. The procedure shown in Figure 6, was used to simulate amine solvents MEA, DEA, and MDEA, in order to capture the carbon dioxide from flue gas, utilizing amine concentrations of 10% and 15% for all solvents and circulation rates of 200 and 300 m<sup>3</sup>/h. In addition, the flue gas flow rate, compositions, temperature, and pressure of the flue gas and amine solvents was kept constant through all scenarios, having 20 trays and a 0.5 pressure drop from the bottom to top column.

The flue gas that feed to the absorber had the following specifications: Temperature of 32 °C; pressure of 30 bar; and CO<sub>2</sub> representing 21% of the total components.

Assumptions of steady state model whereby feed composition and materials flows remained the same during the convergence iterations were made, a 20 trays absorber column typical for Amine absorber columns. The limitation of this study is that it focused on typical natural gas-powered plant alone without consideration to fuel-switch between natural gas and other fuels such as Diesel etc., this was to ensure constant flue gas composition from the plant. Other limitations include steady-state analysis considered compared to the transient operations where plant start-up and shut-down generate different flue gas composition. Figure 7 is a schematic diagram of the simple absorber tower used in an amine sweetening system.

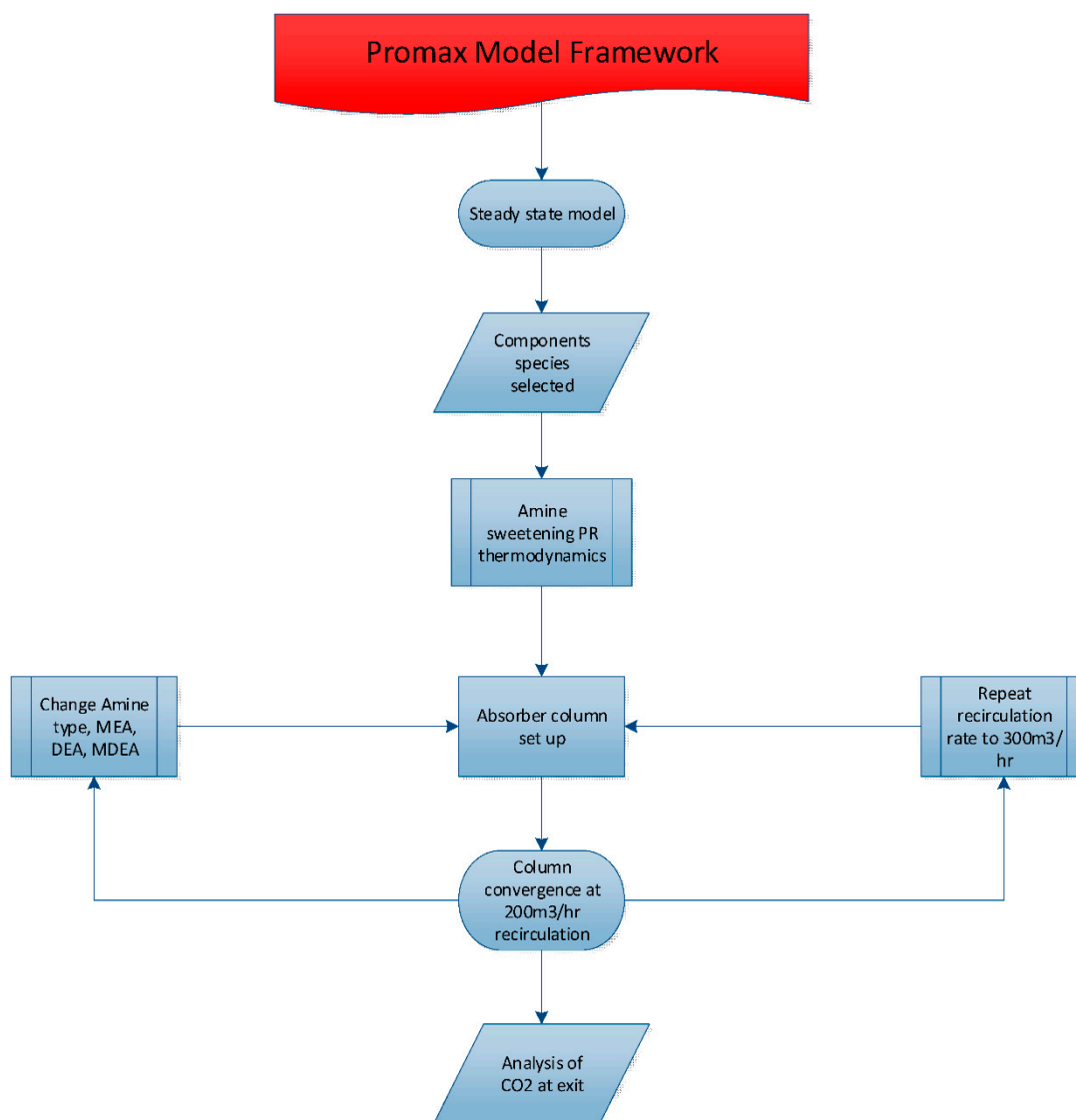


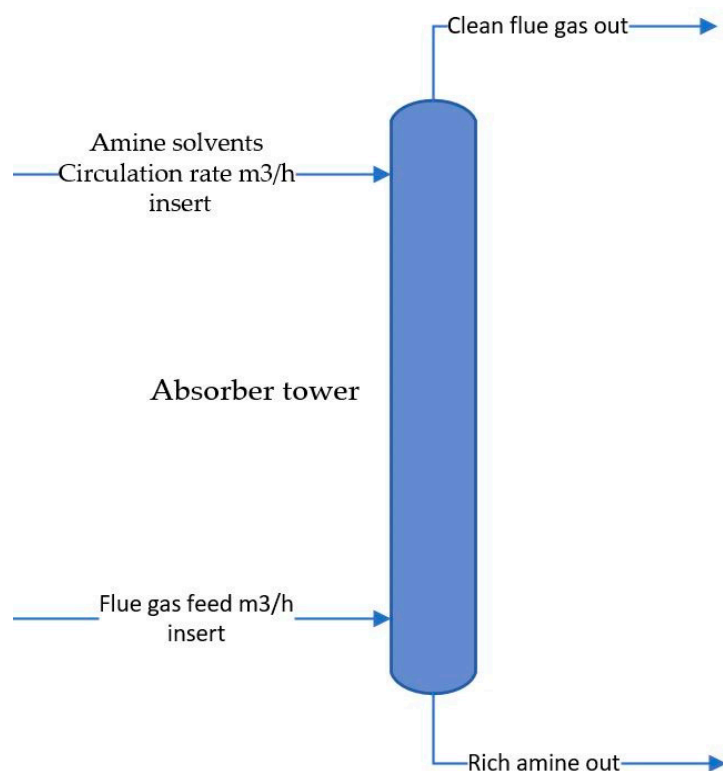
Figure 6. The flow chart of a ProMax simulation.

Tables 7 and 8 show the compositions of flue gas feed and amine solvent, respectively, in mole percentage.

Table 8. Amine-based solution solvents in percent.

Composition of Amine	Mole Percent (%)	
Amine (MEA, DEA and MDEA)	10	15
H <sub>2</sub> O	90	85

With regard to the amine-based solution flow rate, two different flow rates were chosen, which were 200 and 300 m<sup>3</sup>/h for each scenario. The first scenario was a 10% amine concentration of each amine solvent (MEA, DEA, and MDEA) with amine circulation rates of 200 and 300 cubic meters, and the second one was a 15% amine concentration with 200 and 300 m<sup>3</sup>/h. In this chapter, we will investigate the comparison of amine solvents (MEA, DEA, and MDEA) using the ProMax program. This program calculated and solved the process that occurred in the absorber tower and the outcome with an acceptable result.



**Figure 7.** A schematic diagram of the simple absorber tower used in an amine sweetening system.

There are two scenarios for this process, which was conducted by simulations, and some constants did not change during all scenarios:

1. Absorber tower had 20 trays with 29.5 and 30 bar at the top and bottom of the tower pressure;
2. The amine circulation temperature was 38 °C, with a pressure of 33 bar;
3. The flue gas flow rate was 76,000 m<sup>3</sup>/h and temperature were 32 °C, with a pressure of 30 bar.

The other values changed in the two scenarios:

1. The amine circulation rate was changed from 200 to 300 m<sup>3</sup>/h with a concentration of 10% for all flow rates, and 15%.

## 4. Results

### 4.1. The First Scenario

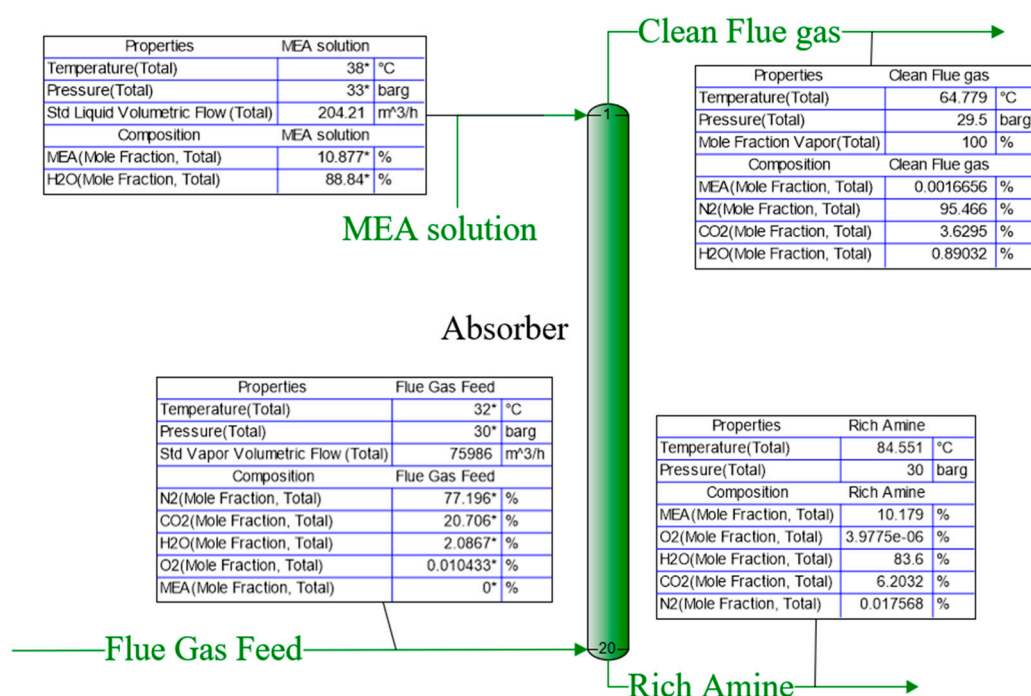
The first scenario for amine solvents MEA, DEA, and MDEA is a concentration of 10% of each solvent with a change in the circulation each time, that which means that 200, 300 m<sup>3</sup>/h that done by simulations of ProMax were conducted with a value of 200 and 300 m<sup>3</sup>/h.

#### 4.1.1. MEA with a Concentration of 10%

MEA with a Circulation Rate of 200 m<sup>3</sup>/h

The whole process that was conducted by ProMax is shown in Figure 8, demonstrating that the resulting products were clean flue gas and rich amine.





**Figure 8.** Absorption process using MEA solvent with a 10% concentration and 200 m³/h simulated by ProMax. “\*” means the results that come out from bottom and top of absorber are mentioned in the Table 9.

**Table 9.** The A summary outcome of the absorber tower results after calculated by ProMax for amine (MEA, DEA, and MDEA) with an amine circulation rate from of 200 and 300 m³/h and with a concentration of 10%, and 15% for each solvent.

Amine Con. wt. %		10%			15%		
Amine Feed	Outcome from Absorber Tower	MEA	DEA	MDEA	MEA	DEA	MDEA
200 m³/h	CO <sub>2</sub> % in clean flue gas	3.6295	8.1355	8.4559	0.0000032862	5.5612	8.2545
	N <sub>2</sub> % in clean flue gas	95.466	91.29	91.278	99.782	93.911	91.51
	Temp. of bottom absorber (°C)	84.551	75.133	73.127	100.75	83.177	75.639
300 m³/h	CO <sub>2</sub> % in clean flue gas	2.9564 × 10 <sup>-6</sup>	0.0038358	3.7518	6.9516 × 10 <sup>-7</sup>	0.00036247	4.305
	N <sub>2</sub> % in clean flue gas	99.768	99.768	96.01	99.782	99.782	95.468
	Temp. of bottom absorber (°C)	78.95	77.21	69.249	83.495	80.638	69.137

#### MEA with a Circulation Rate of 300 m³/h

The whole process that was conducted by ProMax is shown in Figure 9, demonstrating that the resulting products were clean flue gas and rich amine.

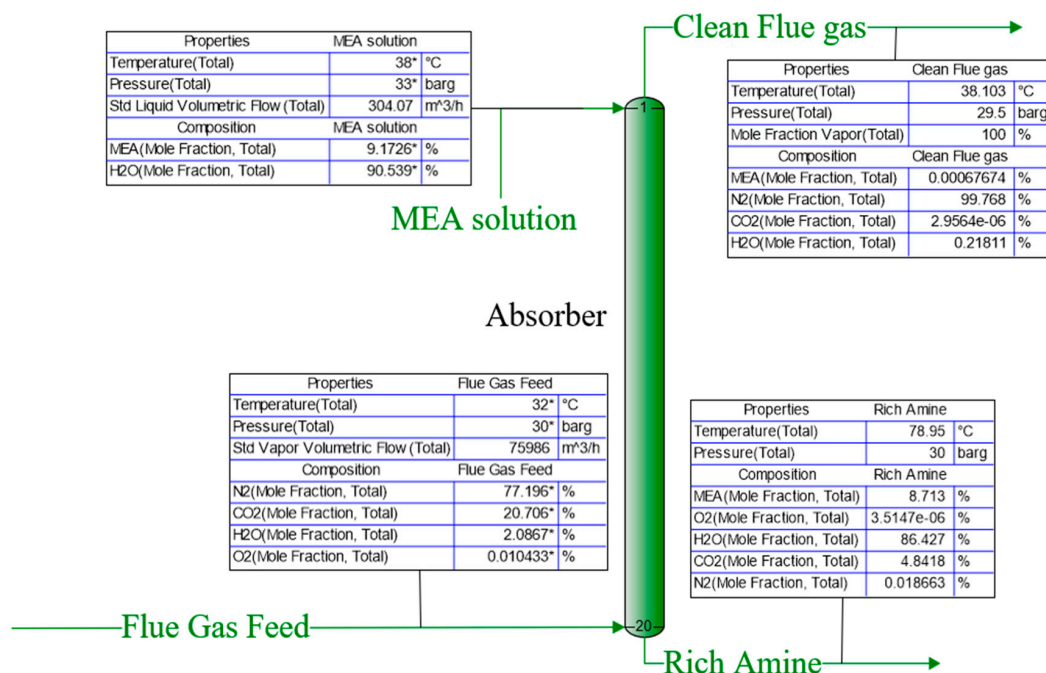


Figure 9. Absorption process using MEA solvent with a 10% concentration and 300 m³/h simulated by ProMax.

#### 4.1.2. DEA with a Concentration of 10%

DEA with a Circulation Rate of 200 m³/h

Using DEA solvent with a circulation rate of 200 m³/h and 10% concentration produced the results shown in Figure 10.

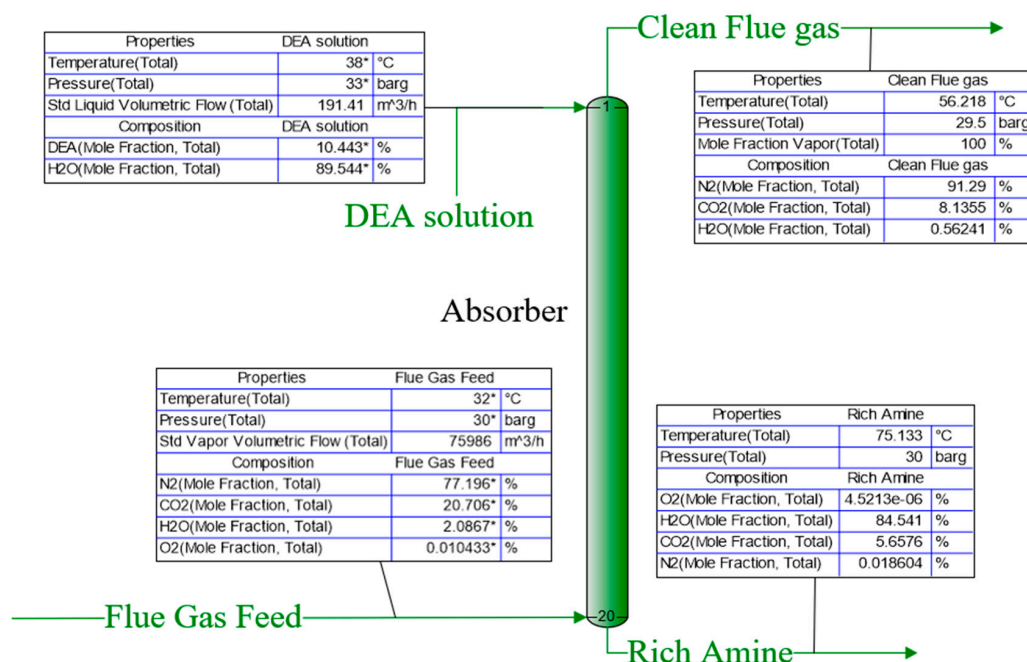


Figure 10. Absorption process using DEA solvent with a 10% concentration and 200 m³/h simulated by ProMax.

DEA with a Circulation Rate of 300 m<sup>3</sup>/h

Using DEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 10% concentration produced the results shown in Figure 11.

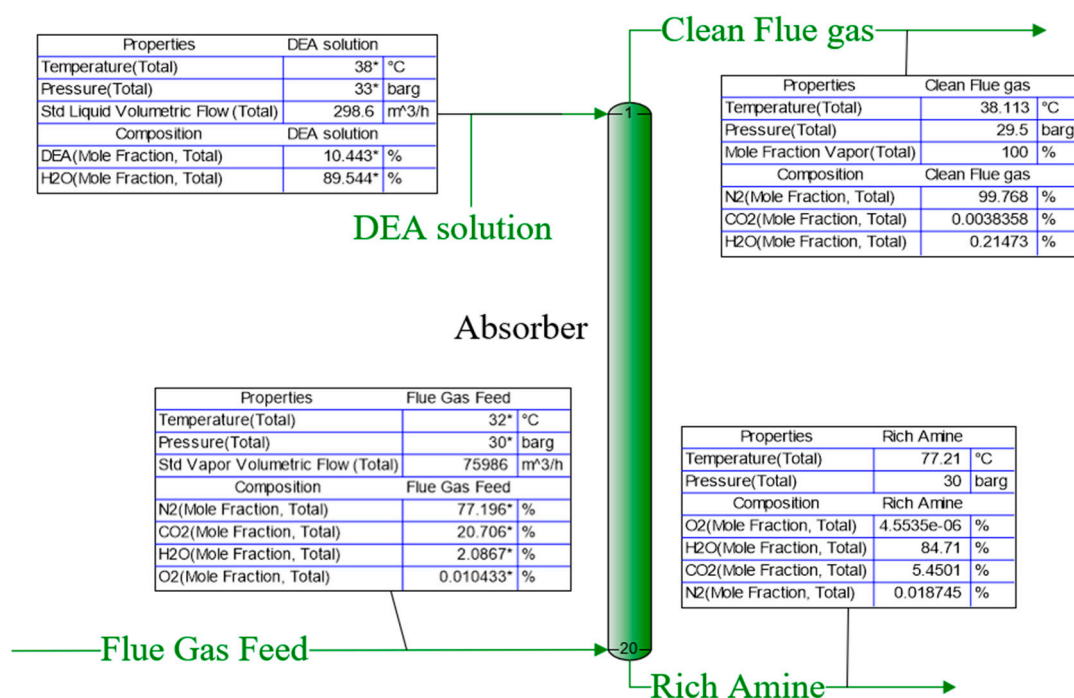


Figure 11. Absorption process using DEA solvent with a 10% concentration and 300 m<sup>3</sup>/h simulated by ProMax.

4.1.3. MDEA with a Concentration of 10%

MDEA with a Circulation Rate of 200 m<sup>3</sup>/h

Using MDEA solvent with a circulation rate of 200 m<sup>3</sup>/h and 10% concentration produced the results shown in Figure 12.

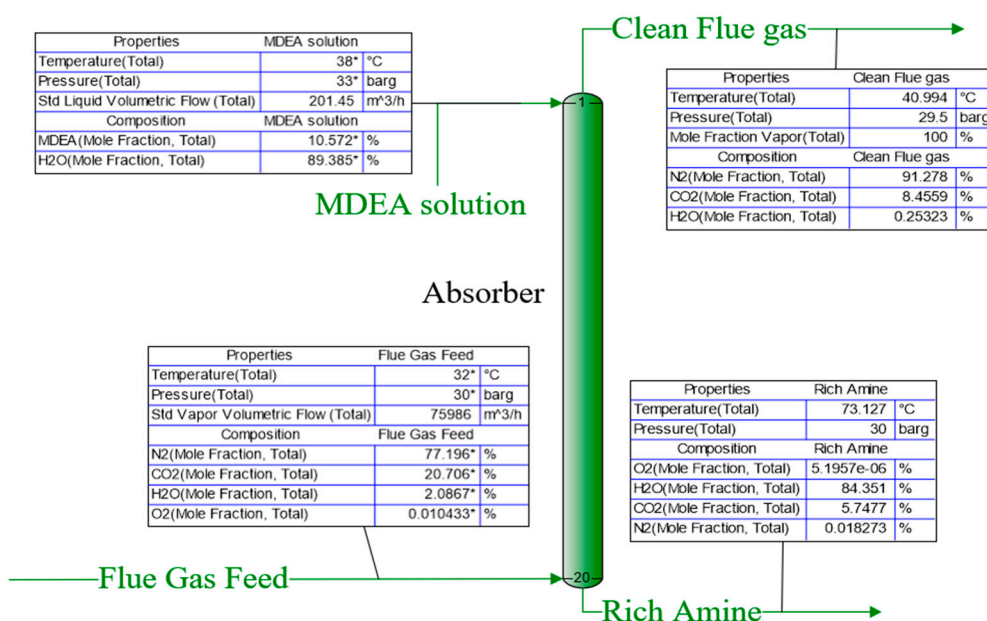


Figure 12. Absorption process using MDEA solvent with a 10% concentration and 200 m<sup>3</sup>/h simulated by ProMax.

MDEA with a Circulation Rate of 300 m<sup>3</sup>/h

Using MDEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 10% concentration produced the results shown in Figure 13.

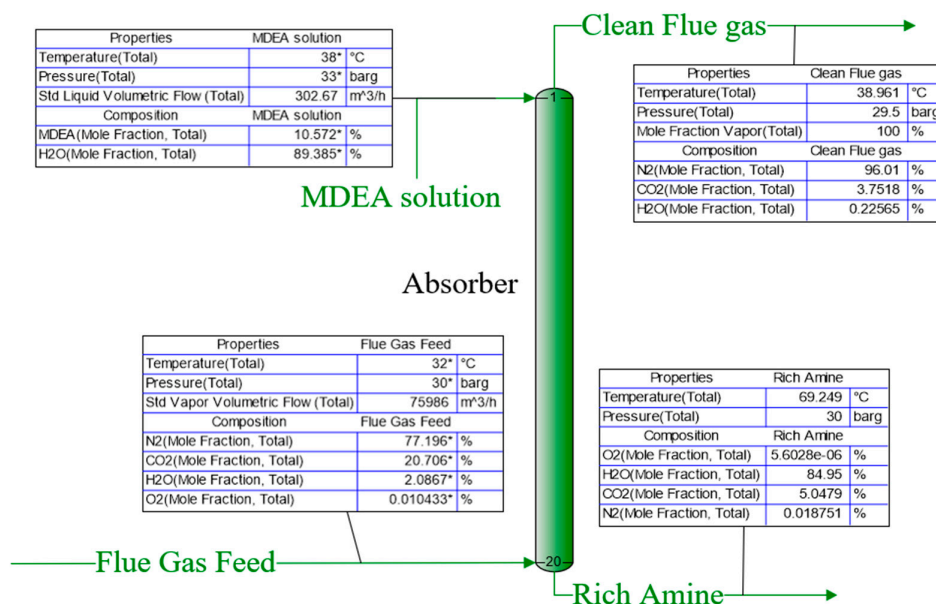


Figure 13. MDEA solvent with a circulation rate of 500 m<sup>3</sup>/h and 10% concentration simulated by ProMax.

#### 4.2. Second Scenario

The second scenario for amine solvents MEA, DEA, and MDEA is was a concentration of 10% of each solvent with a change the circulation each time, that which means that simulations were conducted by ProMax at 200 and, 300 m<sup>3</sup>/h that done by simulations of ProMax.

##### 4.2.1. MEA with a Concentration of 15%

MEA with a Circulation Rate of 200 m<sup>3</sup>/h

Using MEA solvent with a circulation rate of 200 m<sup>3</sup>/h and 15% concentration produced the results shown in Figure 14.

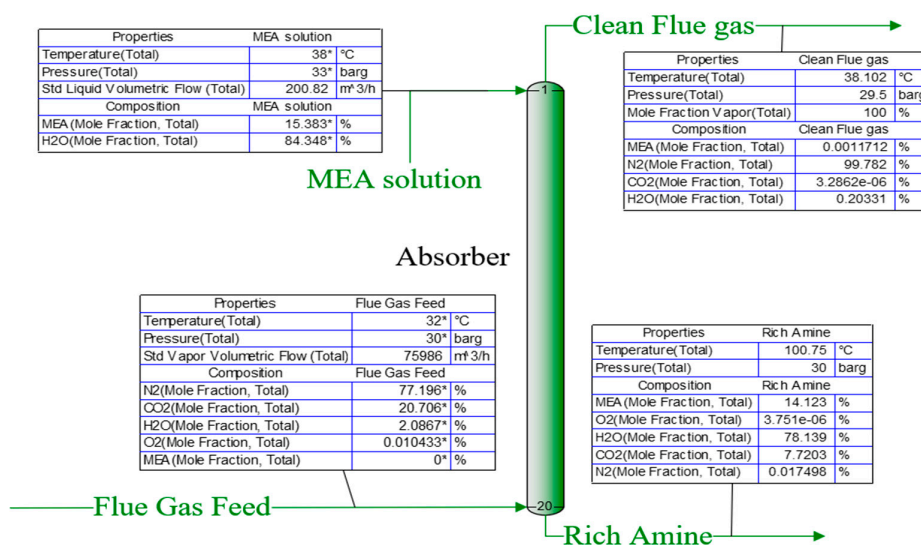


Figure 14. MEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration simulated by ProMax.

MEA with a Circulation Rate of 300 m<sup>3</sup>/h

Using MEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration produced the results shown in Figure 15.

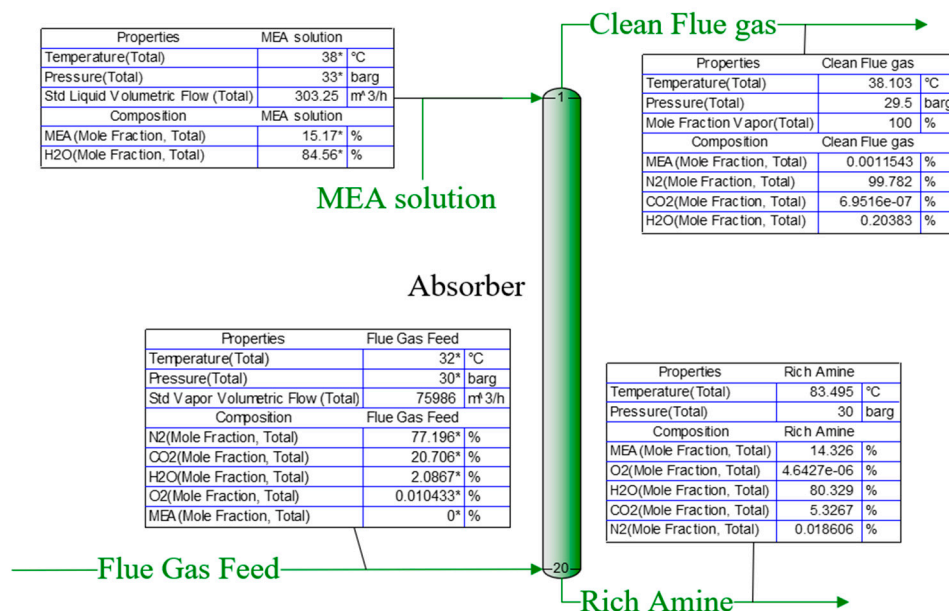


Figure 15. MEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration simulated by ProMax.

4.2.2. DEA with a Concentration of 15%

DEA with a Circulation Rate of 200 m<sup>3</sup>/h

Using DEA solvent with a circulation rate of 200 m<sup>3</sup>/h and 15% concentration produced the results shown in Figure 16.

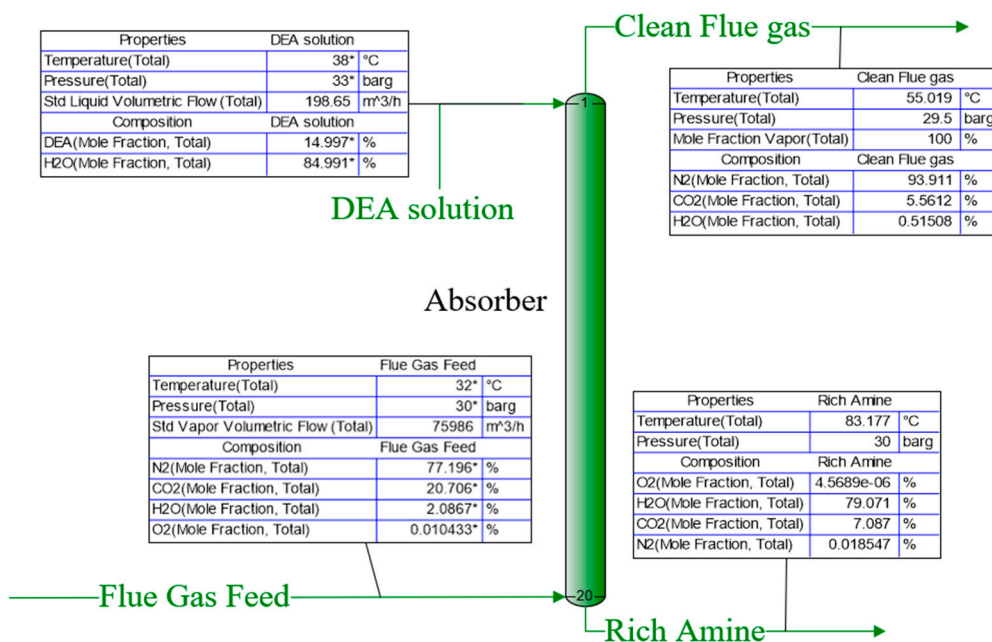


Figure 16. DEA solvent with a circulation rate of 200 m<sup>3</sup>/h and 15% concentration simulated by ProMax.



DEA with a Circulation Rate of 300 m<sup>3</sup>/h

Using DEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration produced the results shown in Figure 17.

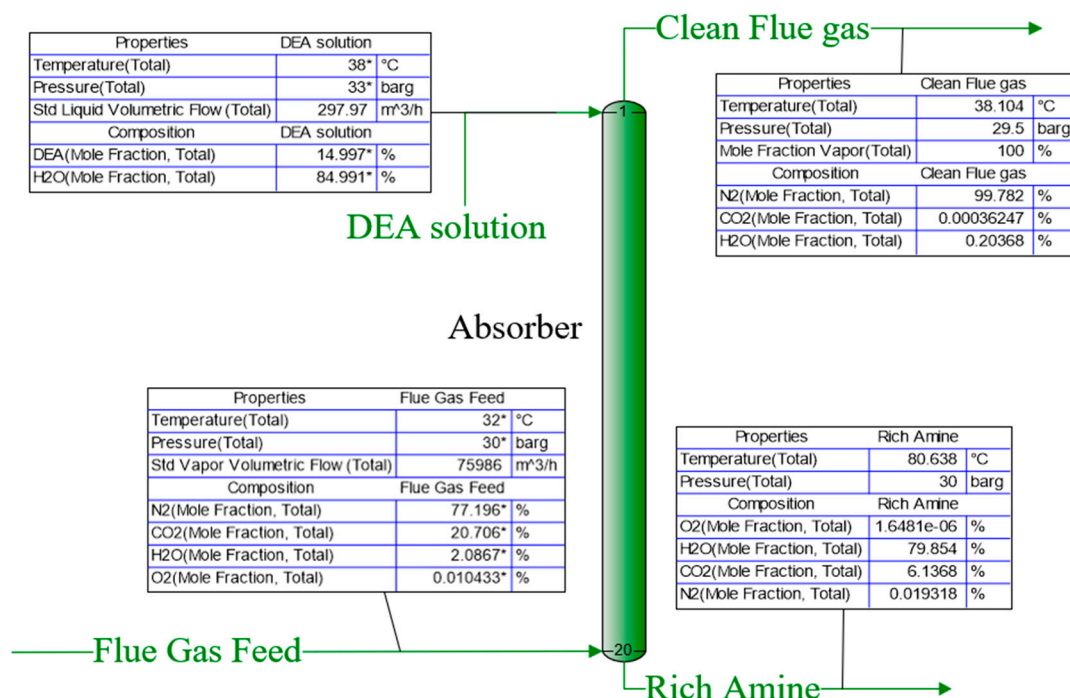


Figure 17. DEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration simulated by ProMax.

4.2.3. MDEA with a Concentration of 15%

MDEA with a Circulation Rate of 200 m<sup>3</sup>/h

Using MDEA solvent with a circulation rate of 200 m<sup>3</sup>/h and 15% concentration produced the results show in Figure 18.

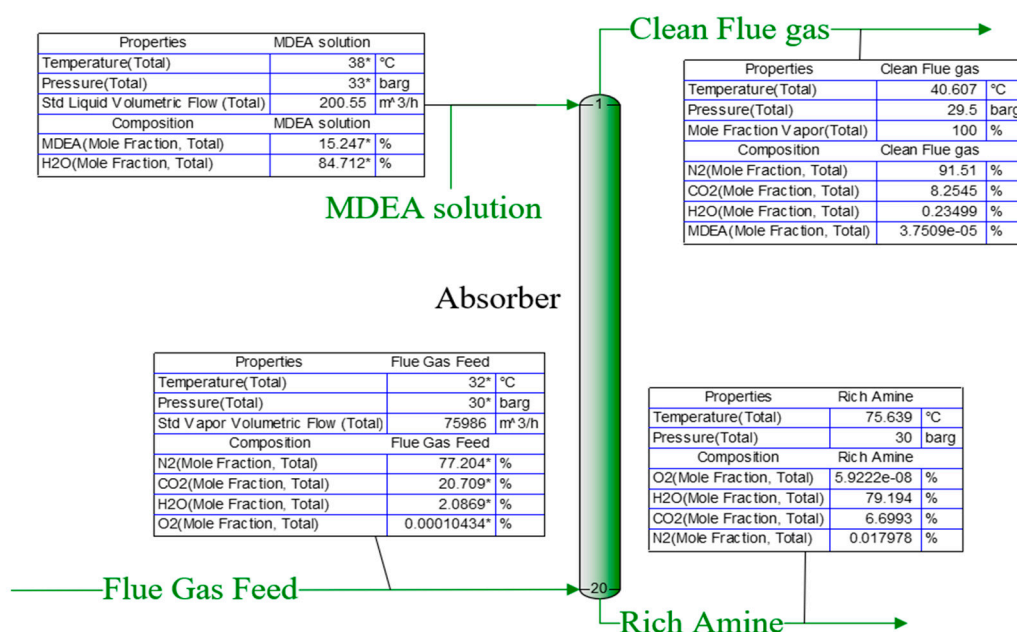


Figure 18. MDEA solvent with a circulation rate of 200 m<sup>3</sup>/h and 15% concentration simulated by ProMax.

MDEA with a Circulation Rate of 300 m<sup>3</sup>/h

Using MDEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration produced the results shown in Figure 19.

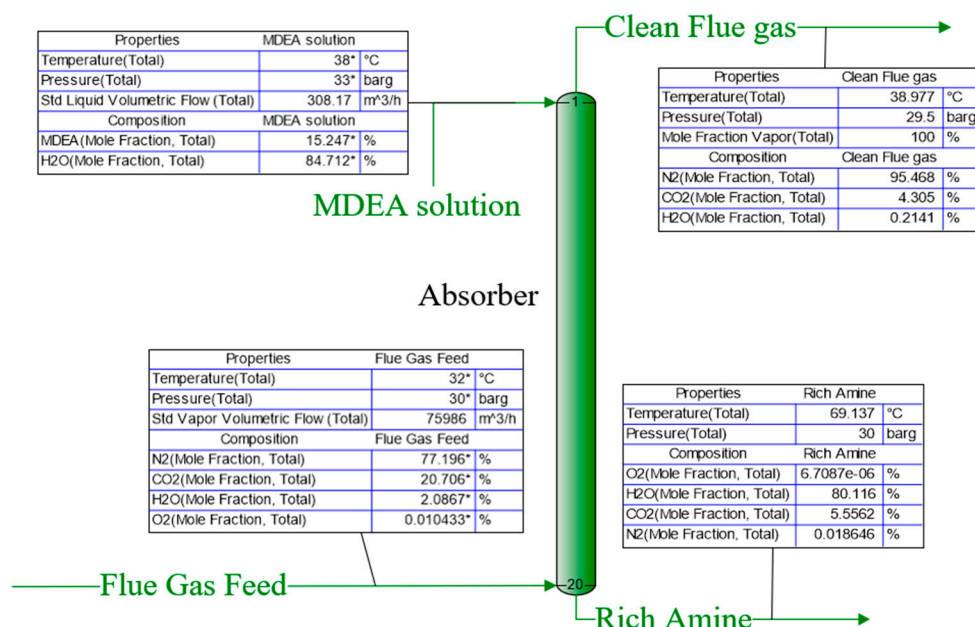
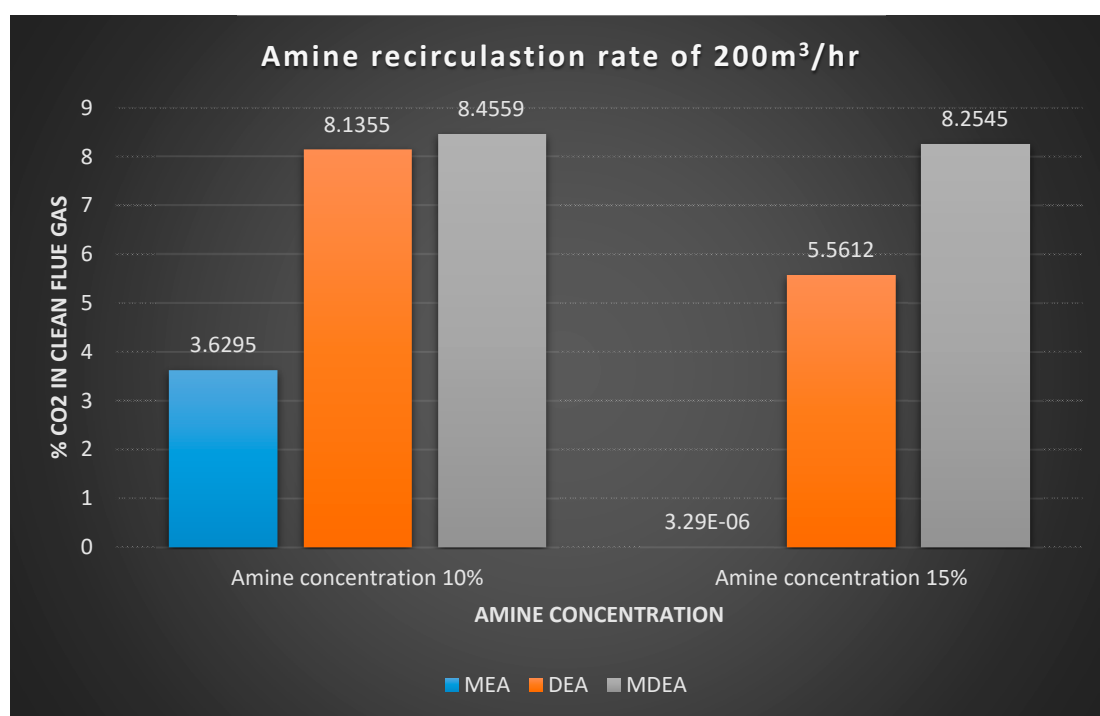


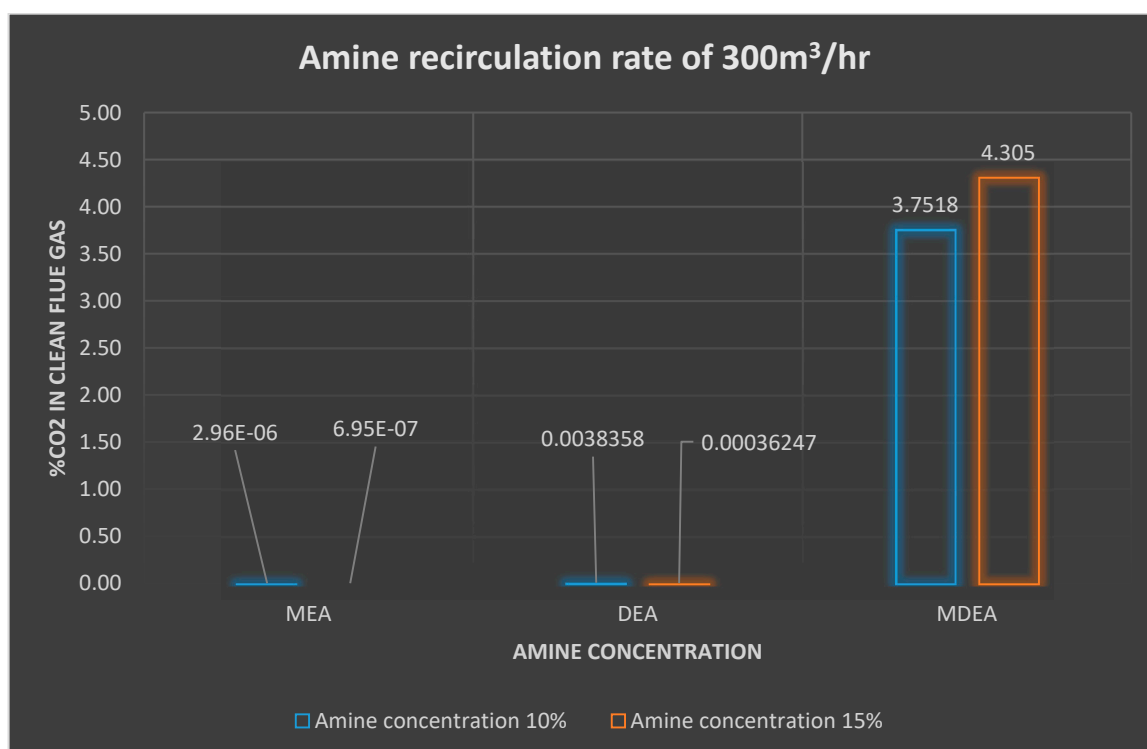
Figure 19. MDEA solvent with a circulation rate of 300 m<sup>3</sup>/h and 15% concentration simulated by ProMax.

A summary of the results obtained from simulations of ProMax was compiled from Figures 8–19 and is shown in Table 9, demonstrating that the MEA solvent is the best solvent in comparison to DEA and MDEA, whilst MDEA is the worst one.

From the aforementioned results presented in Table 9, when using the 200 m<sup>3</sup>/h circulation rate with 10% concentration of amine, the CO<sub>2</sub> % from clean flue gas is 3.6295% for MEA, while that for DEA is 8.1355%. Additionally, that of MDEA is the highest percent, with a value of 8.4559%. Furthermore, at 15%, with the same flow rate mentioned above, DEA and MDEA have the highest percentage values of 5.5612% and 8.2545%, respectively, whilst MEA has a value of  $3.2862 \times 10^{-6}$ %. These mean that the concentration is directly proportional to the flow rate and inversely proportional to CO<sub>2</sub> in the clean flue gas. However, at 200m<sup>3</sup>/h with 10% concentration, the CO<sub>2</sub> in the clean flue gas for MEA is  $2.9564 \times 10^{-6}$ %, while for DEA and MDEA is 0.0038358% and 3.7518%, respectively. At 15% concentration of amine with a circulation rate of 300m<sup>3</sup>/h, the percentage of CO<sub>2</sub> in the clean flue gas for MEA, DEA, and MDEA is  $6.9516 \times 10^{-7}$ %, 0.00036247%, and 4.305%. It has been noted that the percentage of CO<sub>2</sub> in the clean flue gas for MEA and DEA decreased, while for MDEA, at 15% with 300 m<sup>3</sup>/h circulation rate increased. This is because MDEA has different operating condition and it works efficiently from 50 to 60 bars. Another reason is that at this flow (300 m<sup>3</sup>/h) of circulation rate is critical flow and the mass transfer in this flow is false for MDEA. That is the reason why CO<sub>2</sub> % in clean gas flue increased rather than to decreased. As shown in Table 4 the typical concentration should the MDEA be work is 35–55%. Therefore, considering these results, MEA is the best amongst them. Figures 20 and 21 illustrate the CO<sub>2</sub> percent in clean flow gas at 200 and 300 m<sup>3</sup>/h for MEA, DEA and MDEA at 10 and 15% concentration of amines.



**Figure 20.** The CO<sub>2</sub>% in clean flue gas with concentration of amine solvents (MEA, DEA, and MDEA) at 200 m<sup>3</sup>/h.



**Figure 21.** The CO<sub>2</sub>% in clean flue gas with concentration of amine solvents (MEA, DEA, and MDEA) at 300 m<sup>3</sup>/h.

#### 4.3. The Cost of Amine

To find out which solvent costs the least, each one's price was estimated by performing a calculation. The result shows that the MEA is the best solvent. The prices were as follows:

- (a) GBP 1121/ton for monoethanolamine (MEA) [33];
- (b) DEA GBP 1039/ton [33];
- (c) MDEA unknown?
- (d) To calculate the price, there should be a specific gravity for amine to convert the cubic meters to tons, as shown in Equations (11) and (12);
- (e) Specific gravity of MEA = 1.01531, density = 1015.31 kg/m<sup>3</sup> = 1.01531 t/m<sup>3</sup> (Pro-Max program):

$$\text{Total MEA ton} = \text{Amine feed} \times \text{Amine concentration\%} \times \text{Density (ton/m}^3\text{)} = \text{ton} \quad (11)$$

$$\text{Total cost} = \text{Total MEA ton} \times \text{GBP/ton} = \text{GBP} \quad (12)$$

Therefore, by using Equations (11) and (12), the cost was calculated and is shown for MEA in Table 10 and for DEA in Table 11.

**Table 10.** The total weight of amine (MEA) in tons, with the total cost in GBP.

MEA Solution m <sup>3</sup> /h	10% = Net MEA Tons from Solution	Total Cost GBP (GBP 1121/ton)
200	20.3062	22,763.25
300	30.4593	34,144.88

**Table 11.** The total weight of DEA in ton with total cost in GBP.

DEA Solution m <sup>3</sup> /h	10% = Net DEA Tons from Solution	Total Cost GBP (GBP 1039/ton)
200	20.8718	21,685.8002
300	31.3077	32,528.7003

- (a) Specific gravity of DEA = 1.04359, density = 1043.59 kg/m<sup>3</sup> = 1.04359 t/m<sup>3</sup> (Pro-Max program).

The capital cost for CO<sub>2</sub> capture facility is USD 223 million and capture cost (USD/tonne CO<sub>2</sub>) ranges between USD \$36–70 for MEA for a typical gas-powered power plant integrated with Carbon capture using MEA shown in Table 12 [19,34].

**Table 12.** The cost of MEA for one a real company for post capture of CO<sub>2</sub>.

Study	[19,34]
Industrial source	Combined stack gas
CO <sub>2</sub> capture technology	PCC MEA
CO <sub>2</sub> capture efficiency (%)	90
CO <sub>2</sub> captured (Mt CO <sub>2</sub> /y)	1.04
Project life (years)	20
Currency	US
Cost year	2007
External power plant or fuel	Natural gas
Capital cost for capture facility (millionUSD)	223
Capture cost (USD/tonne CO <sub>2</sub> avoided)	36–70

## 5. Conclusions

From the present study, the following conclusions can be drawn:

1. From the results of Table 9, it can be concluded that
  - At 10% concentration and feed of 200 m<sup>3</sup>/h of amine solvents, the outcome obtained cannot be chosen for capture because the CO<sub>2</sub>% in flue gas for each

MEA, DEA and MDEA are 3.6295%, 8.1355%, and 8.4559%, respectively, and these values are not enough. With these percentages obtained my target was not achieved neither of other of other researchers because to use capture process there should be clear from CO<sub>2</sub>% in clean flue gas as aforementioned is not acceptable (the percentage of carbon dioxide) as sustainable for power plants, even the temperature at the bottom of the absorber is quite good but the purity of nitrogen is not qualified to be utilized to other purposes such as food processes.

- MEA produces a good outcome at 200 m<sup>3</sup>/h with a 15% concentration in comparison to DEA and MDEA, with their values being  $3.2862 \times 10^{-6}$ , 5.5612, and 8.2545, respectively, but the temperature of the rich amine is still high, so it is recommended that cooling is induced by increasing the flow rate or decreasing the concentration of amine;
  - Likewise, the MEA has perfect significant results at a 300 m<sup>3</sup>/h amine circulation rate at a 10% concentration, reducing the temperature to 78.95 °C, whereas the temperature was 100.75 °C at 15%. A good result of 77.21 °C was obtained for 0.0038358% of CO<sub>2</sub> in the top outlet of the tower and 99.768% nitrogen for both MEA and DEA and 96.01% for MDEA, with 3.7518% CO<sub>2</sub> in clean flue gas, which is still high, however, the other significant advantages of capturing CO<sub>2</sub> is that the gained nitrogen, with a purity 99.68%, can be used for other purposes;
  - For MDEA, the bad result means that the operating condition needs to be changed, which changes the pressure to 50 or 60 bar. This will produce good results but will be costly.
2. Based on the results in Tables 10 and 11, the following comparison can be drawn:
    - For MEA at 200 and 300 m<sup>3</sup>/h, the total weight in tons was equal to 20.3062 and 30.4593, with a total cost of GBP 22,763.25 and 34,144.88, respectively;
    - for DEA at 200 and 300 m<sup>3</sup>/h, the total weight in tons was equal to 20.8718 and 31.3077, with a total cost of GBP 21,685.8002 and 32,528.7003, respectively.
  3. Finally, from the results of the comparison, MEA was proven to be the best solvent investigated in this study, rather than DEA and MDEA; however, the DEA was slightly cheaper than MEA, but the result was an enormously different comparison with MEA.

**Author Contributions:** S.H. conducted the study simulation and data analysis, A.J.A. supervised the overall research, contributed to paper development and editing, G.G.N. conducted review and made changes to the manuscript. All authors have read and agreed to the published version of the manuscript.

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## Abbreviations

BP	British Petroleum
IPCC	Intergovernmental on climate change
CCS	Carbon capture and storage
CO <sub>2</sub>	Carbon dioxide
COS	Carbonyl sulfide
SO <sub>2</sub>	Sulfur dioxide
NO <sub>x</sub>	Nitrogen oxides (x = 1, 2, 3)
O <sub>2</sub>	Oxygen
N <sub>2</sub>	Nitrogen
H <sub>2</sub> O	Water or (vapor water)



H <sub>2</sub> S	Hydrogen sulfide
PM	Particulate matter
RDF	Radial distribution functions
MEA	Monoethanolamine
DEA	Diethanolamine
DGA	Diglycolamine
MDEA	Methyldiethanolamine
DIPA	Diisopropanolamine
TIPA	Triisopropanolamine
Gt	Gigatons
Mt	Million tons
MPa	Megapascal (unit of pressure)
Ppm	Part per million
PCC	Post-combustion capture

### Appendix A

pKa: This is one method that can be used to indicate the strength of acid.  $pK_a = -\log_{10}K_a$  means  $pK_a$  is a negative logarithm of the  $K_a$  value. In addition, a higher  $pK_a$  value indicates a weaker acid, and a lower value of  $pK_a$  means a stronger acid, and the latter means that the acid is fully dissociated in water.

Dimers: A structure implicates two similar or identical units. These units may be associated by noncovalent forces or covalent bonding [31].

Rich amine: An amine solution that has held or absorbed the acid gas CO<sub>2</sub> from the flue gas during the absorption process.

Lean amine: An amine solution that does not contain any acid gas CO<sub>2</sub> and this means that, before the absorption processes, the amine undergoes the regeneration process, which removes all acid gas, producing a lean amine.

**Table 1.** The properties of CO<sub>2</sub> that used in amine absorption come out from ProMax simulation program.

Properties		
	Units	Vapor
Temperature	°C	32
Pressure	barg	30
Mole fraction vapor	%	100
Mole fraction light liquid	%	0
Mole fraction heavy liquid	%	0
Molecular weight	Kg/kmol	44.0095
Mass density	Kg/m <sup>3</sup>	65.0285
Molar flow	Kmol/h	2272.24
Mass flow	Kg/h	100,000
Vapor volumetric flow	m <sup>3</sup> /h	1537.79
Liquid volumetric flow	m <sup>3</sup> /h	1537.79
Normal vapor volumetric flow	Nm <sup>3</sup> /h	50,929.8
Std vapor volumetric flow	m <sup>3</sup> /h	53726.7
Std liquid volumetric flow	m <sup>3</sup> /h	121.773
Compressibility		0.827261
Specific gravity		1.51953
API gravity		
Enthalpy	KJ/h	$-8.96706 \times 10^8$
Mass enthalpy	kJ/kg	−8967.06
Mass Cp	kJ/(kg °C)	1.08707
Ideal gas Cp, Cv ratio		1.28541
Dynamic viscosity	cP	0.0166239
Kinematic viscosity	cSt	0.25564
Thermal conductivity	W/(m °C)	0.0198344
Surface tension	dyn/cm	
Net ideal gas heating value	MJ/m <sup>3</sup>	0
Net liquid heating value	MJ/kg	−0.17659
Gross ideal gas heating value	MJ/m <sup>3</sup>	0
Gross heating value	MJ/kg	0.17659

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